D-Alanine, N-(2-chlorobenzoyl)-, hexadecyl ester

Inchi: InChI=1S/C26H42ClNO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-18-21-31-26(30)22(2)28-2
InchiKey: DKUDKKJVWDJVAY-UHFFFAOYSA-N
Formula: C26H42ClNO3
SMILES: CCCCCCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccccc1Cl
Mol. weight [g/mol]: 452.07

Physical Properties

Property code	Value	Unit	Source
gf	-17.00	kJ/mol	Joback Method
hf	-679.84	kJ/mol	Joback Method
hfus	66.91	kJ/mol	Joback Method
hvap	102.74	kJ/mol	Joback Method
log10ws	-9.01		Crippen Method
logp	7.483		Crippen Method
mcvol	384.670	ml/mol	McGowan Method
pc	915.50	kPa	Joback Method
rinpol	3377.00		NIST Webbook
rinpol	3377.00		NIST Webbook
tb	1043.26	K	Joback Method
tc	1279.72	K	Joback Method
tf	611.39	K	Joback Method
vc	1.492	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1301.25	J/mol×K	1043.26	Joback Method
cpg	1317.70	J/mol×K	1082.67	Joback Method
cpg	1332.64	J/mol×K	1122.08	Joback Method
cpg	1346.18	J/mol×K	1161.49	Joback Method
cpg	1358.39	J/mol×K	1200.90	Joback Method
cpg	1369.38	J/mol×K	1240.31	Joback Method
cpg	1379.22	J/mol×K	1279.72	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354083&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume